

Vol. 17, No. 6, November-December 2023

EDITORIAL 153

Review Articles

Computational Identification of Novel TMPRSS2 Inhibitors for COVID-19
Therapeutics

Molecular modeling of doping agents and their metabolites for potential pharmacological activity assessment

CRIPS Digest 179

BUSINESS CORRESPONDENCE

Enquiries concerning advertisements should be addressed to the Editorial Office CRIPS.

Published by National Institute of Pharmaceutical Education and Research (NIPER), S.A.S. Nagar (Punjab)

No part of this publication may be reproduced, copied or transmitted in any form without prior permission of the publisher.

EDITORIAL OFFICE

National Institute of Pharmaceutical Education and Research (NIPER), Sector 67, S.A.S. Nagar - 160062 (Punjab), INDIA

Tel.: 0172-2292000,2214682

E-mail : crips@niper.ac.in web : www.niper.gov.in

DISCLAIMER:

The opinions & views expressed by the authors in CRIPS belong to authors but not to Publishers. While every care has been taken in the preparation of CRIPS, the publishers are not responsible for such opinions and views or for any inaccuracy in the articles. Also it is expected that the authors checked the articles for plagiarism.

The cover page contains a figure from the article of Dr. Devendra Kumar Dhaked

EDITORIAL

The SARS CoV-2 infection started in Dec 2019, and caused more than 7 million deaths worldwide. Vaccines have been developed by pharmaceutical companies, including two Indian companies. However, there are reports of SARS CoV-2 infection of vaccinated people. There is a necessity of new drug development for treatment of COVID-19. The virus uses ACE2 receptor for cell entry, and followed by interaction with TMPRSS2. TMPRSS2 is a protein present on plasma membrane of host cell. Development of TMPRSS2 inhibitors could be a potential strategy for the treatment of COVID-19. The screening of more than 1 million compounds from Asinex and Otava libraries found 135 ring structures. Further MD studies predicted that nine compounds possess higher binding free energy compared to Nafamostat (-31.1 kcal/mol).

Athletes use nutraceuticals and other drug substances to improve their physical activities, competitiveness. A few of them may have side effects such as dependency, psychotropic effects, cardiovascular, respiratory problems. Those are considered as dopants. The World Anti-Doping Agency (WADA) continuously monitors the levels of dopants. WADA has published a list of prohibited substances, it is monitored by national agencies (e.g., the National Anti-doping Agency (NADA) and its laboratories National Dope Testing Laboratory (NDTL). The drugs like etilefrine (an agonist of the $\alpha 1$ and $\beta 1$ adrenergic receptors), to emifene (antiestrogenic, selective estrogen receptor modulator), ethylmorphine (a narcotic used to reduce pain) are used by athletes and these are banned by WADA. Molecular docking studies of doping agents and their metabolites with their respective biological targets shows that the binding affinities of metabolites are similar to the parent compounds except for an norethylmorphine and o-dephenyl ostarine. ADME analysis of dopants and their metabolites were evaluated, and norethylmorphine, etilefrine sulfate and carboxy toremifene might retain a portion of the parent dopant's pharmacological actions.

Dr. Sharada Prasanna Swain

Editor-In-Chief

Prof. Prasad V. Bharatam, NIPER, S.A.S. Nagar

Associate Editors

Prof. Gopabandhu Jena, NIPER, S.A.S. Nagar

Prof. Ipsita Roy, NIPER, S.A.S. Nagar Dr. Joydev Laha, NIPER, S.A.S. Nagar

Dr. Chandraiah Godugu, NIPER, Hyderabad Dr. Sharada P. Swain, NIPER, Kolkatta

Business Correspondance

Dr. Srikant Bhagat, NIPER, S.A.S. Nagar

Publication Editor

Dr. Vishnu K. Sharma, NIPER, S.A.S. Nagar

Layout & Design

Mr. Promod Kumar, NIPER, S.A.S. Nagar

Distributions & Publicity

Mr. Amit Thapar, NIPER, S.A.S. Nagar